Atomistic Design and Simulations of Nanoscale Machines and Assembly
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Prof. William A. Goddard III
Dr. Tahir Cagin
Materials and Process Simulation Center (MSC),
Caltech, Pasadena California
Dr. Stephen P. Walch,
Eloret Corp.,
Mountain View, California

1.0 Accomplishments

Over the three years of this project, we made significant progress on critical theoretical and computational issues in nanoscale science and technology, particularly in:

- Fullerenes and nanotubes
- Characterization of surfaces of diamond and silicon for NEMS applications
- Nanoscale machine and assemblies
- Organic nanostructures and dendrimers
- Nanoscale confinement and nanotribology
- Dynamic response of nanoscale structures nanowires (metals, tubes, fullerenes)
- Thermal transport in nanostructures

Projects completed include (in each case papers have been published and the results presented at national conferences):

1. Molecular Mechanics and Molecular Dynamics Studies of alkali doped Single Walled Nanotubes [1]
2. Characterization of SWNTs and Tori with accurate (QM derived) Force Fields using molecular mechanics [2]
3. Molecular Dynamics and Molecular Mechanics Simulations of Nanomachines [3]
4. Extensive Quantum Mechanical (QM) studies of diamond mechano-synthesis [4]
5. *Generalization of Empirical Bond Order Dependent Potentials:* Development of EBOP with terms to represent long range tube-tube interactions in a continuous manner to address nano and micro tribology problems for nano-mechanical and micro mechanical devices. The problems of wear and friction are especially important in the design of nano- or micro-mechanical devices for long term space mission [5].
6. *Molecular Self-Assembly:* The tribology of molecularly thin self-assembled layers and their influence on friction and wear. We considered heterogeneous systems composed of surfaces

(mostly hard materials), physisorbed or chemisorbed organic molecularly thin layers on these surfaces, and the fluid interfaces. [6-8]

7. *Supramolecular Assembly:* The convergent and divergent synthetic methods developed for dendrimers have substantial potential in the design of tailored hyperbranched structures for use in molecular nanotechnology applications. We studied the structure and properties of these systems and the self-assembly of dendrimers on surfaces as possible nano- or micro scale sensor applications. [9-11]
8. *Transport Properties of Carbon Nanotubes:* Nanotubes for nano electronic device components are being studied experimentally by numerous researchers at various labs. For development of nanoelectronic devices, an essential issue to be addressed is the thermal transport properties of carbon nanotubes. Over the past two years, we developed non-equilibrium molecular dynamics techniques to study the transport properties of materials. These methods employ synthetic fields to generate currents and to measure the response of materials. Our earlier applications centered on mass transport (diffusion) and flow properties (viscosity) for fluids. In the third year, we studied the thermal conductivity of nanotubes, fullerenes, and diamond using molecular dynamics. The calculated thermal conductivities are found in good agreement with the experiment using the new generalized empirical bond order potentials [12, 13].
9. *Inherent Tribological Properties of Nanoscale Materials:* At present, silicon forms the basis of microelectronic and Microelectromechanical devices (MEMS). However, silicon has inherently poor wear properties whereas single crystal diamond and polycrystalline diamond have excellent tribological properties if properly protected by chemisorbed hydrogen. The promising developments in carbon nanotube synthesis and application make carbon-based materials attractive for device design. Using advanced quantum mechanical techniques, we investigated the H_2 –Si and H_2-C interactions [14]. We also used bond order dependent potentials in MD to study the friction and wear of diamond (100) surfaces for NEMS and MEMS applications [15, 16]
10. *Failure Mechanisms in Nanotubes*: Using NEMD techniques and bond order dependent force fields for Carbon, we investigated the failure of nanotubes as a function of strain rate [17].
11. *Plasticity and deformation behavior of metallic nanowires*: Using the steady state MD methods (nonequilibrium MD), we studied the deformation behavior of metallic nanowires [18, 19]. We found that the deformation mechanisms involved twin generation rather than the dislocation creation characteristic of micron and larger systems.
12. *Metals in low dimensions*: We used many-body Force Fields to study the properties of nanoscale thin films, nano-wires, and nano-dots [20]. We characterized the decrease in melting temperature and other properties for nanoscale systems
13. *Formation of fullerenes and nanotubes:* Using ab initio density functional methods and the new reactive force fields, we determined the mechanism of the formation for fullerenes, and nanotubes [21].

The computational nanotechnology effort at the Materials and Process Simulation Center is described in detail in a review article, which appeared in the inaugural issue of the Journal of Nanoparticle Research [22]. Another review article is in preparation of the multiscale modeling and simulation methods and application in nano tribology [23].

2.0 Education, training and outreach

Over the three years of this project a number of graduate students (Dr. G. Gao, Y. Qi, G. Wang, R. Martin, G. Zamanakos, P. J. Miklis, W. Deng, and Lu Sun) and undergraduate students (N. Breen), and postdoctoral fellows (Dr. Jianwei Che, Dr. Yanhua Zhou) have worked on these projects. Visiting scholars included

- Prof. Hideyuki Ikeda from Japan and Prof. Konrad Samwer from Germany, who focused on the characterization of metallic nanowires, their phase transformations and deformation behavior,
- Dr. Andres Jaramillo-Botero who focused on nanoscale machines.

The research results have been incorporated into Chemistry 121, the computational materials chemistry course given each year at Caltech. This has introduced the Caltech undergraduate and graduate students to nanoscale science and technology.

Publications List

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14. S. P. Walch, W. A. Goddard, III, and T. Cagin, Computational Studies of the Interaction of H/H2 with Diamond and Silicon Surfaces presented at the 1998 Foresight Conference on Molecular Nanotechnology (1998).
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